# ML FOR CHEMISTRY AND MATERIALS

CyberTraining Workshop and Summer School 2026

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University at Buffalo
Department of Chemical and Biological Engineering
School of Engineering and Applied Sciences

# Acknowledgements

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The State University of New York

# The role of chemical & materials research

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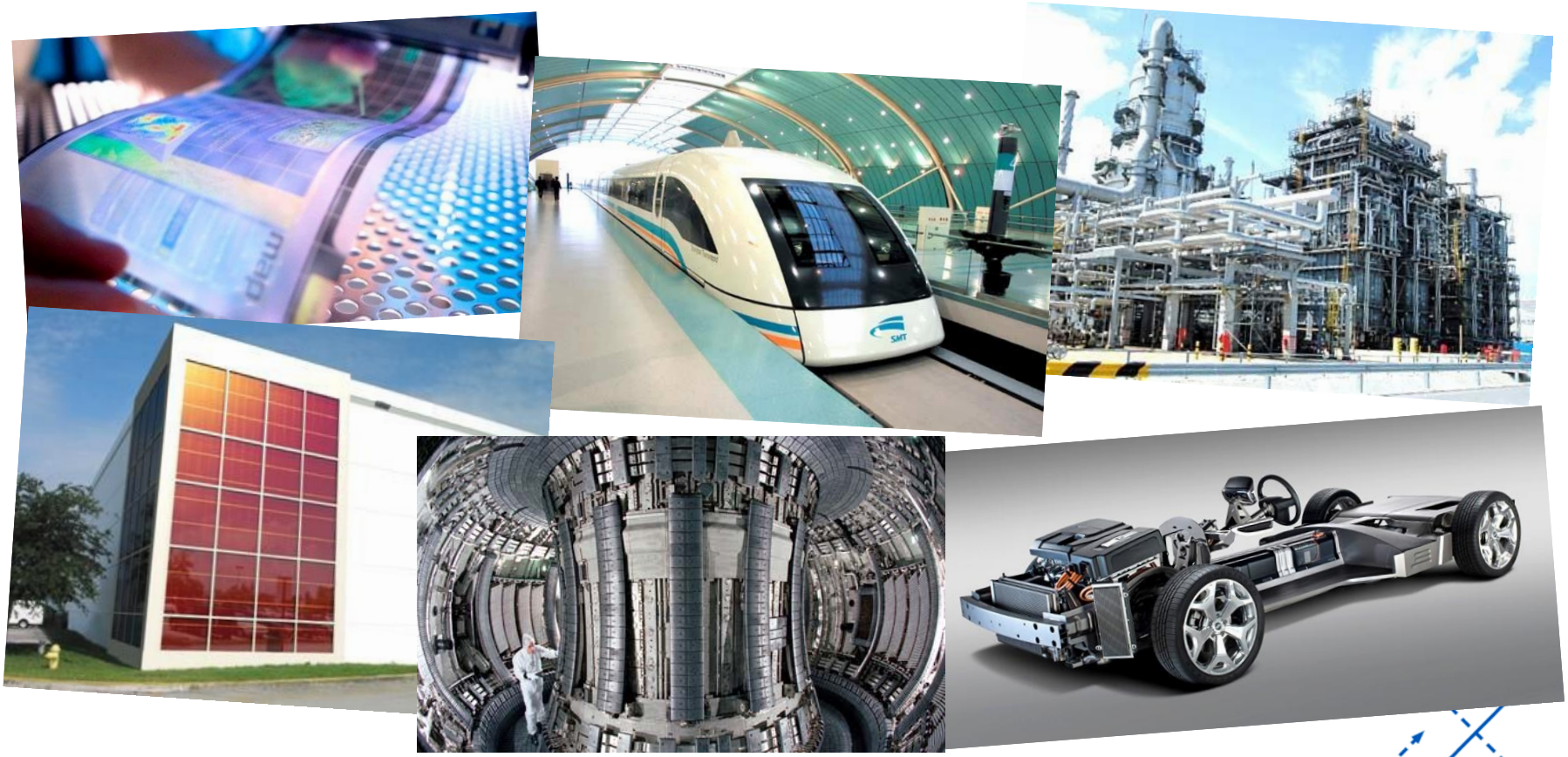
**Real-world solutions** to mankind's **grand challenges** in **innovation, energy, and sustainability** can be found in the discovery and development of **novel compounds, processes, and materials**.



# Theory-driven chemical & materials research

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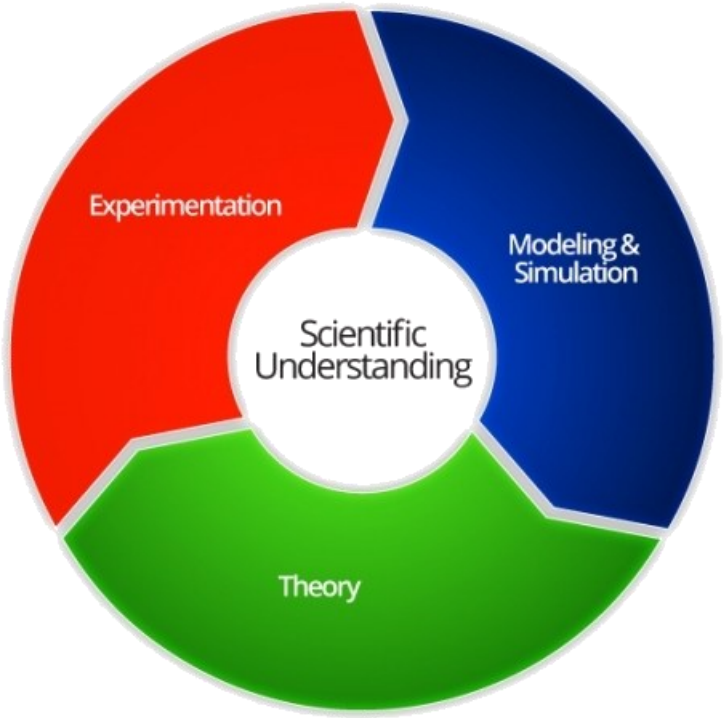
**Real-world solutions** to mankind's **grand challenges** in **innovation, energy, and sustainability** can be found in the discovery and development of **novel compounds, processes, and materials**.

- **progress** increasingly **driven by physics-based modeling, simulation** (QC, MD, ...)




DOE

# Theory-driven chemical & materials research

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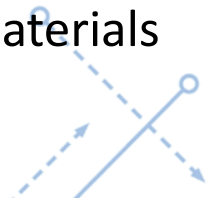
**Real-world solutions** to mankind's **grand challenges** in **innovation, energy, and sustainability** can be found in the discovery and development of **novel compounds, processes, and materials**.

➢ **progress** increasingly **driven by physics-based modeling, simulation** (QC, MD, ...)

- computational studies are **efficient** means to **uncover promising targets** for more time- and resource-intensive investigations in the lab
- they can significantly **accelerate** research by making **guiding predictions**
- they can **provide unique insights** beyond the scope of empirical observation and thus contribute a solid foundation to new findings

➢ <u>thus:</u> they are a valuable asset for **synergistic** research in chemistry, materials



# Data-driven chemical & materials research

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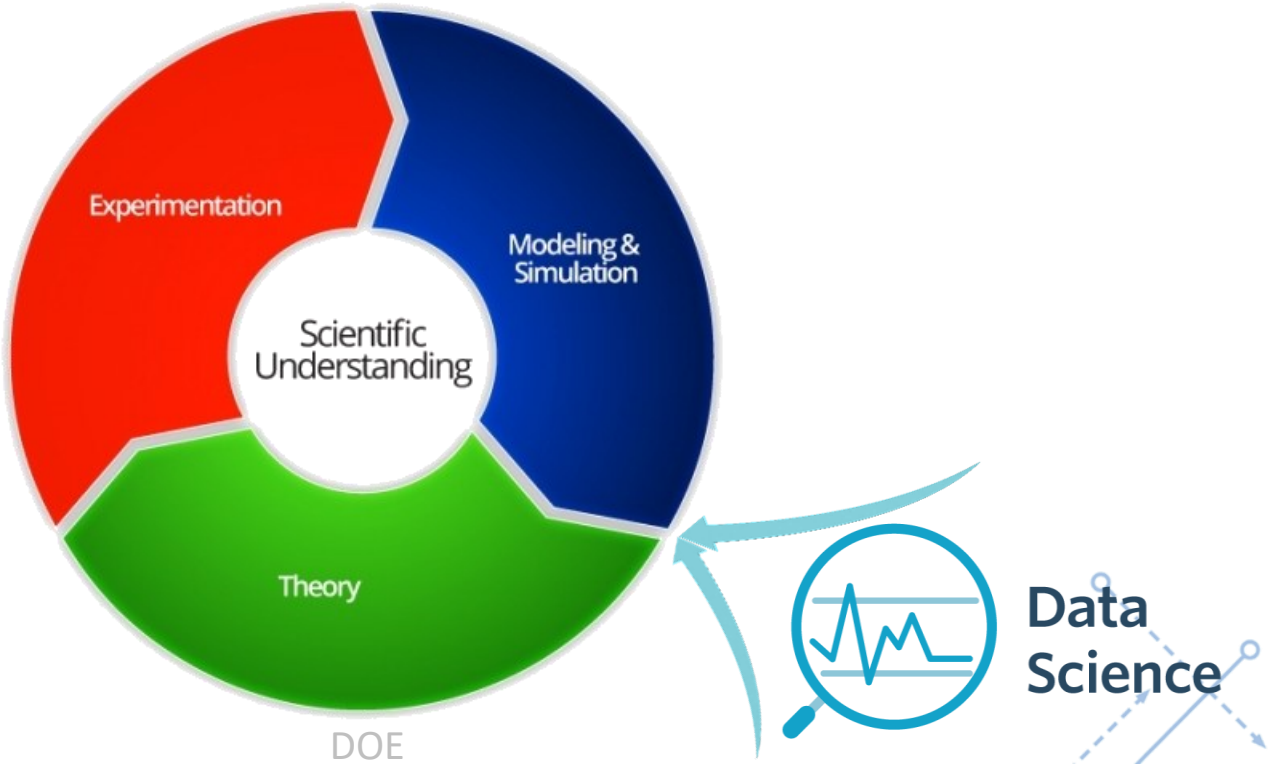
**Real-world solutions** to mankind's **grand challenges** in **innovation, energy, and sustainability** can be found in the discovery and development of **novel compounds, processes, and materials**.

- **progress** increasingly **driven by physics-based modeling, simulation** (QC, MD, ...)
- rise of **data-driven** approaches: "*4th pillar of science*"

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# Data-driven chemical & materials research

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- **progress** increasingly **driven by physics-based modeling, simulation** (QC, MD, ...)
- rise of **data-driven** approaches: "*4th pillar of science*"
  - VHTS, CI/MI, DM, ML, DL, AI, …

- automated/autonomous VHTS allows for **large-scale *in silico* exploration of chemical space** (its uncharted domains may hold new compound classes with **transformative properties**)
  - generates large data sets

- DM, ML, DL: extract insights, patterns from data sets, create prediction models

# 2011 White House Materials Genome Initiative

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# 2017 Data-Driven Discovery Science in Chemistry

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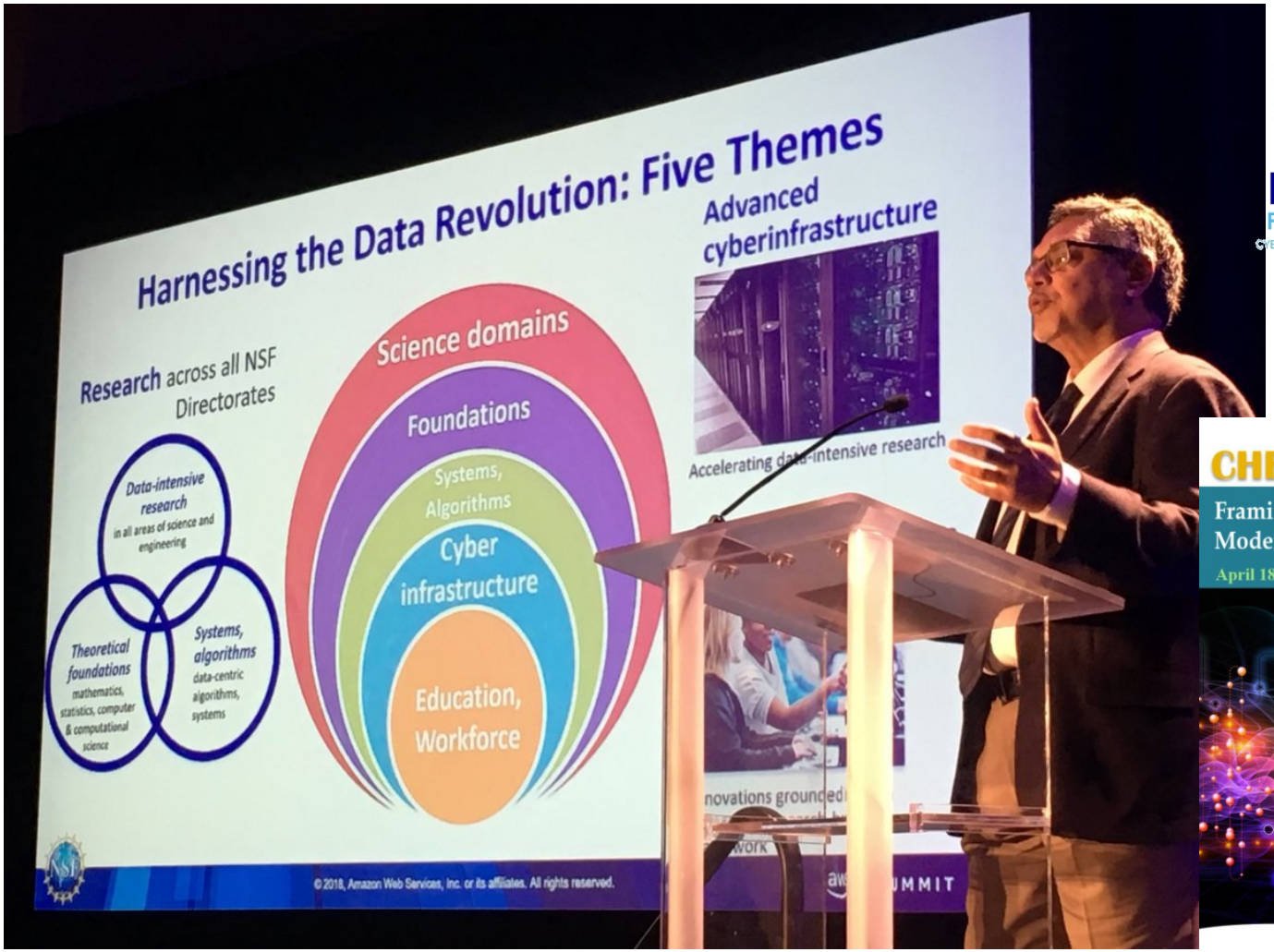



# AI *vs* ML *vs* DL

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- ML: techniques to generate data-derived prediction models (surrogate models)

# AI *vs* ML *vs* DL

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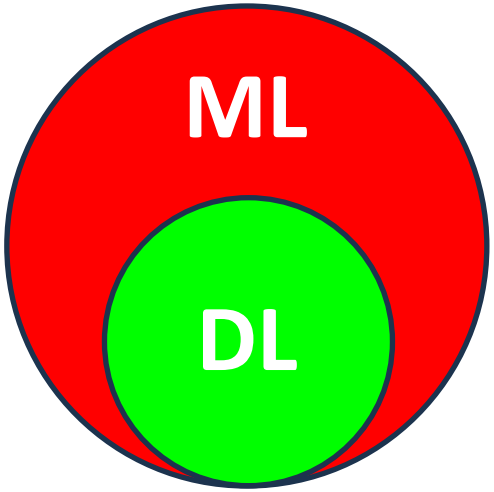
- DL: a particular class of ML algorithms (using multi-layer neural networks)



# AI *vs* ML *vs* DL

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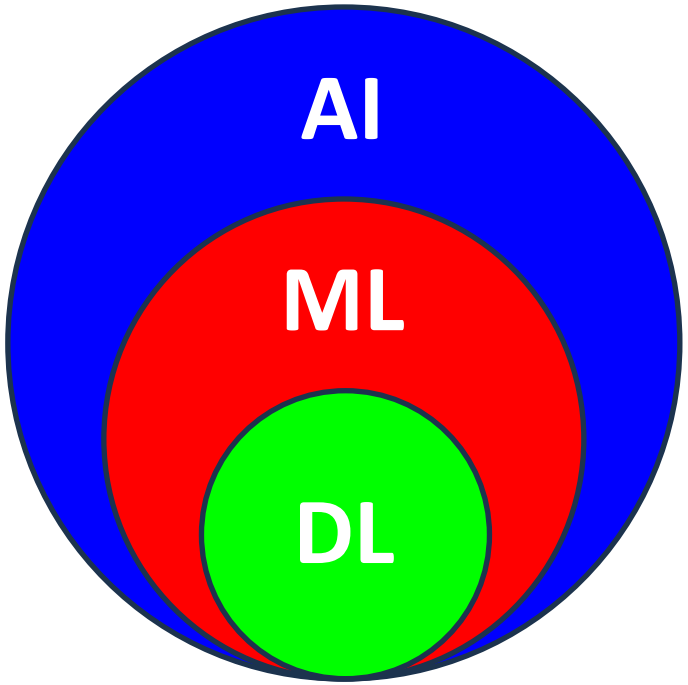
- ML: techniques to generate data-derived prediction models (surrogate models)
- DL: a particular class of ML algorithms (using multi-layer neural networks)
- AI: techniques to interact with ML models in a human-like fashion



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# PHYSICS-BASED *VS* DATA-DERIVED MODELS

What's the difference?

# Physics-based models

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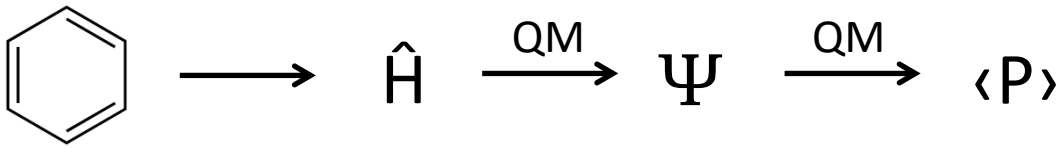
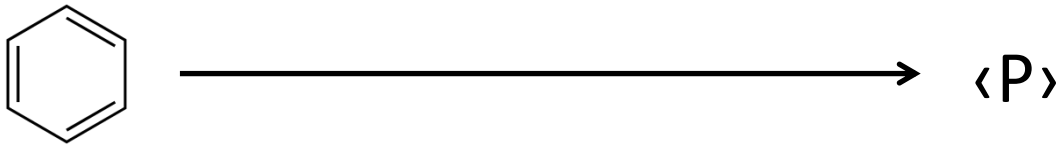
- physics (e.g., QM) rigorously maps a structure to a property




  - i.e., there exists a structure-property causality
  - BUT: QM is **expensive**, we want to recover mapping more efficiently
  - BUT: QM is **opaque**, we want to identify relevant aspects of SPR

  - … could there be a shortcut?






*COChE* 23 (**2019**), 51.

# Data-derived models

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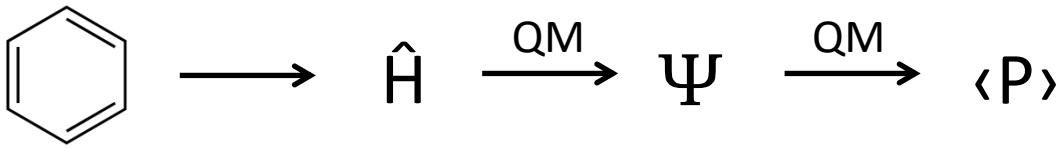
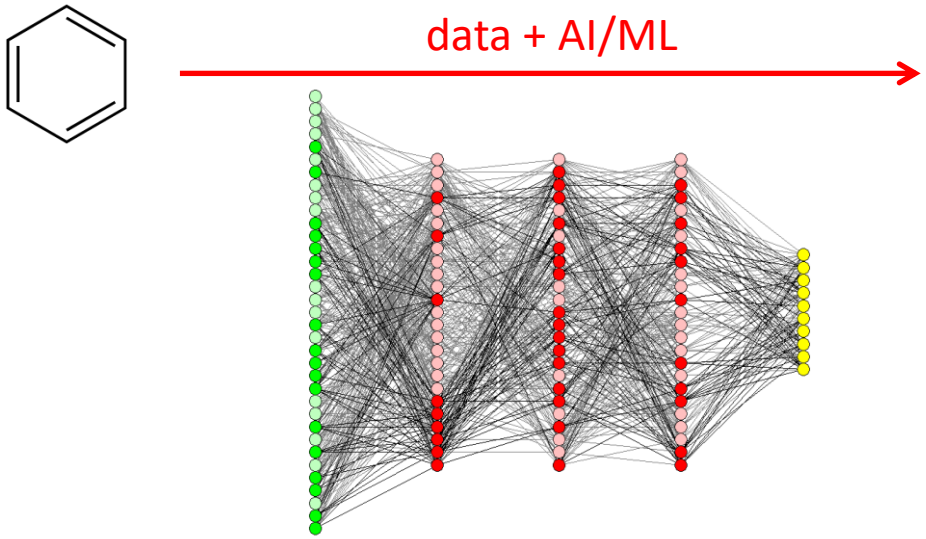
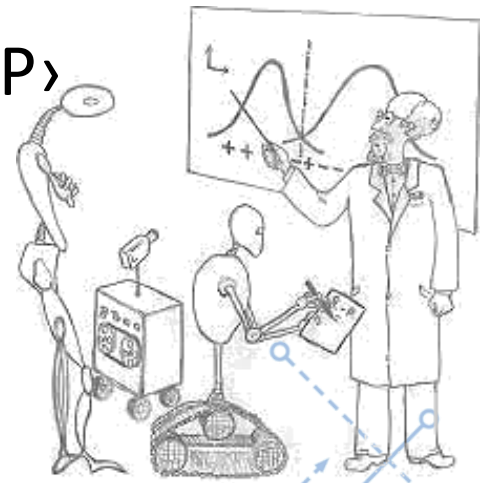



  - i.e., there exists a structure-property causality
  - BUT: QM is **expensive**, we want to recover mapping more efficiently
  - BUT: QM is **opaque**, we want to identify relevant aspects of SPR

  - … could there be a shortcut? *Yes, via AI/ML!*



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# Data-derived models

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| | property |
|---|---|
| n compounds | … <br> $p_n$ <br> … |

- goal: create prediction model based on set of experimental/computational data



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# Data-derived models

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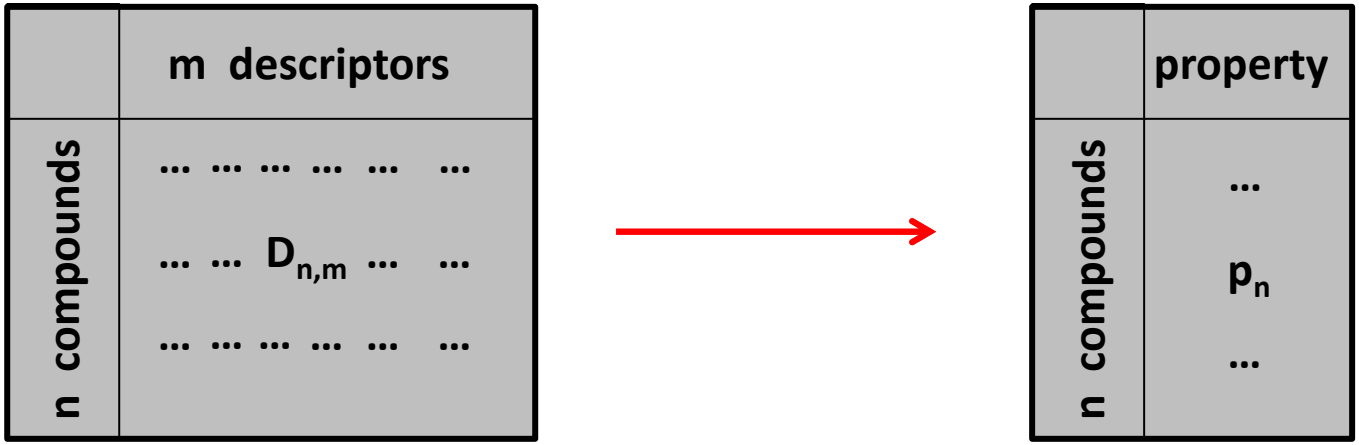


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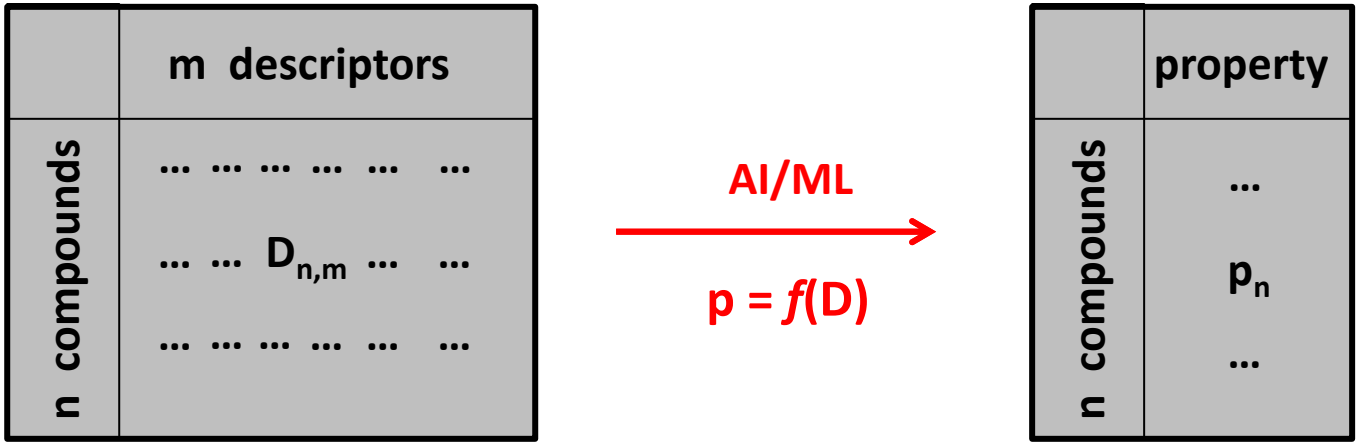
# Data-derived models




- goal: create prediction model based on set of experimental/computational data

- ***f*** is **predictive**, encapsulates essence of **structure-property relationships!**
- we can use ***f*** for **HTP discovery,** $f^{-1}$ for **rational design, inverse engineering!**

- ***f*** is easy to evaluate, allowing for **fast results!**



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# A WORKING EXAMPLE

Discovery and design of
high-refractive index polymers

# Ex: Development of high-refractive-index polymers

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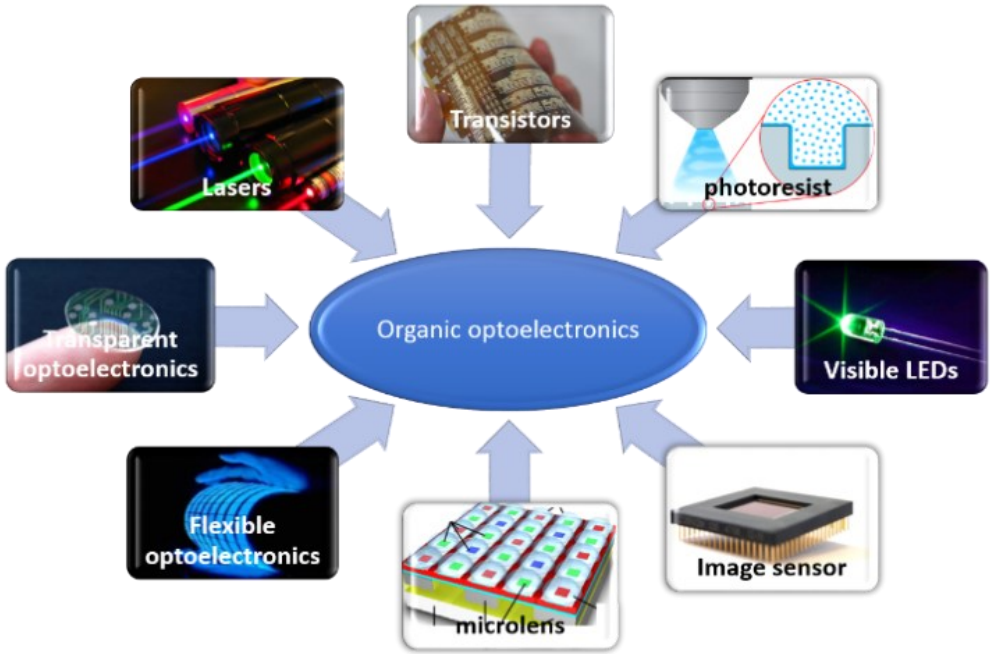
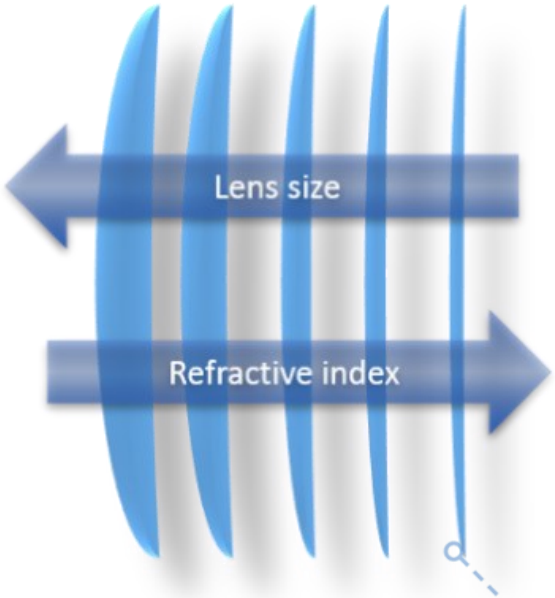
- plastic material for **optic, optoelectronic applications**:
  - anti-reflective coatings, optical adhesives, substrates for advanced displays, micro-lenses in image sensors
  - *in situ* application
- <u>problem:</u> RI > 1.7 needed, but typical C-based polymers have RI ≈ 1.3 to 1.5






*JCP* 148 (**2018**), 241712; *JPCC* 123 (**2019**), 14610; *PCCP* 21 (**2019**), 4452.

# Ex: Development of high-refractive-index polymers

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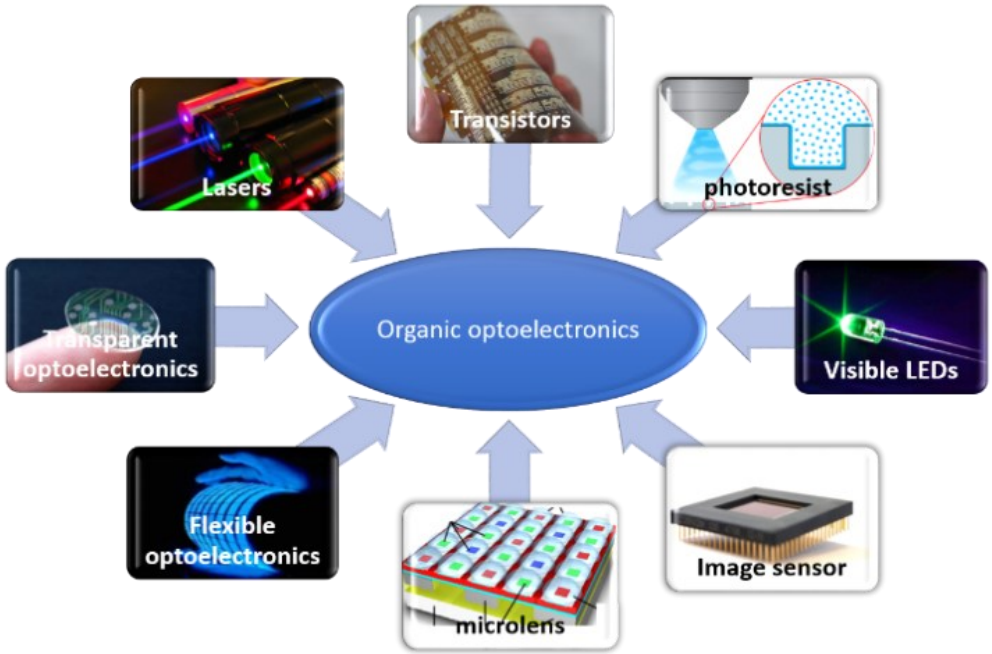
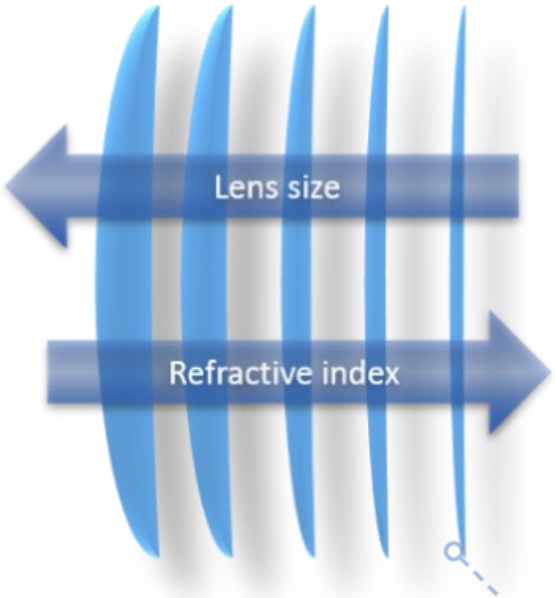
**Lorentz-Lorenz equation**:
(Clausius-Mossotti relation)

$$n_r = \left(\frac{1 + 2\boldsymbol{\alpha}\,\mathbf{N}/3\epsilon_0}{1 - \boldsymbol{\alpha}\,\mathbf{N}/3\epsilon_0}\right)^{1/2}$$



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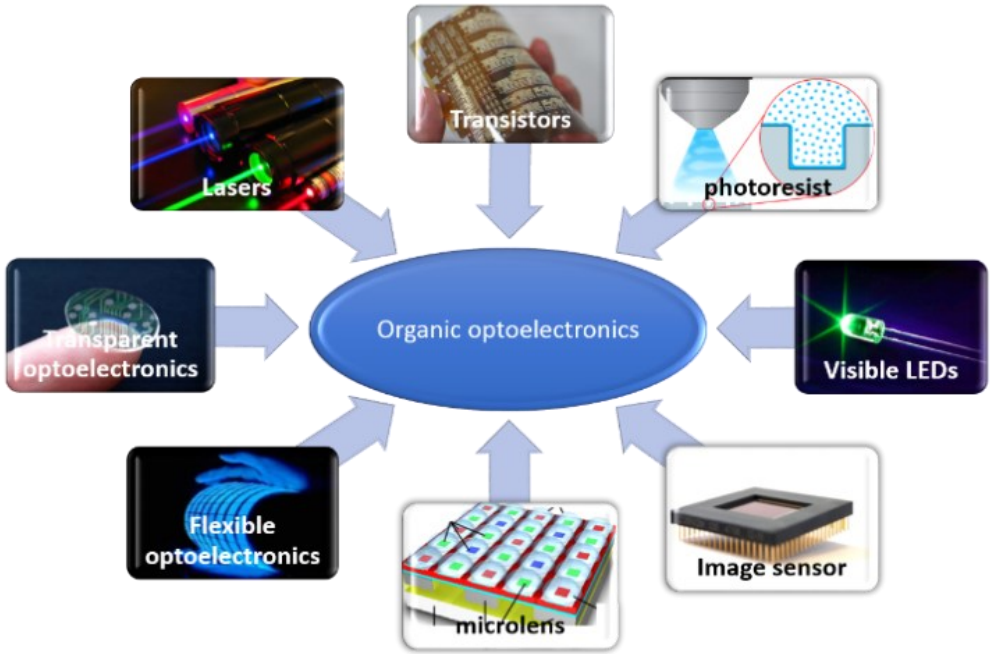
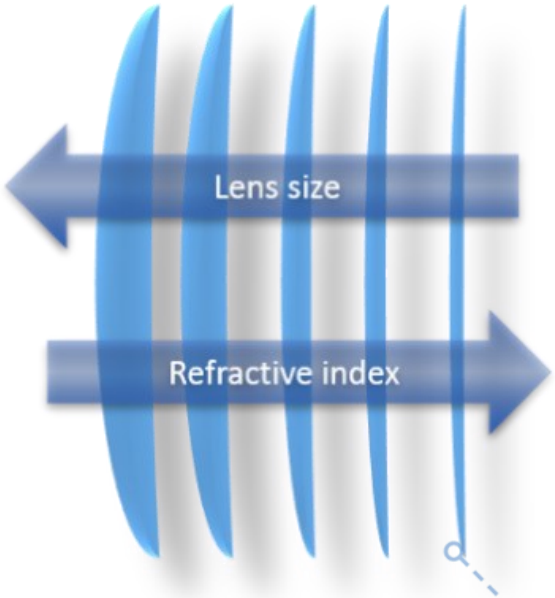
refractive index — molecular polarizability — number density



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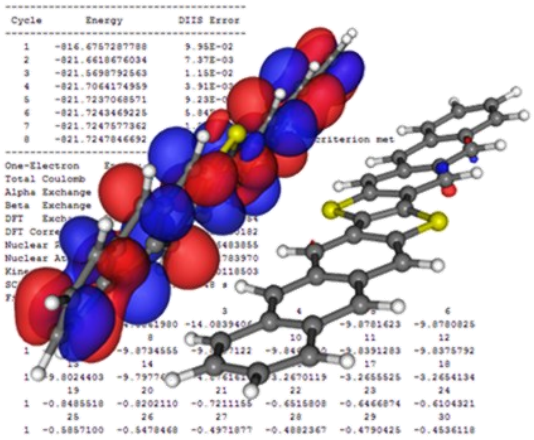
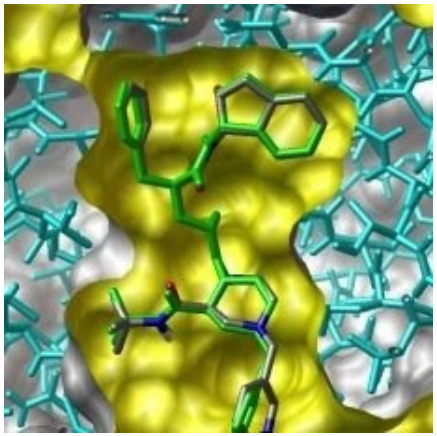
**refractive index**

**molecular polarizability (e.g., from DFT)**

**number density (e.g., from MD)**







*JCP* 148 (**2018**), 241712; *JPCC* 123 (**2019**), 14610; *PCCP* 21 (**2019**), 4452.

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# A WORKING EXAMPLE

Replace physics-based
with data-derived models

# Ex: Development of high-refractive-index polymers

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**Lorentz-Lorenz equation**:
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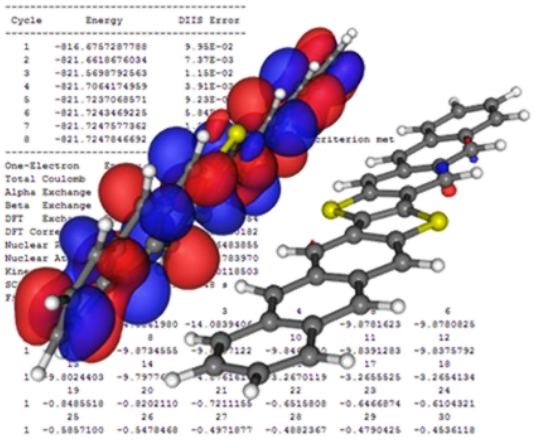
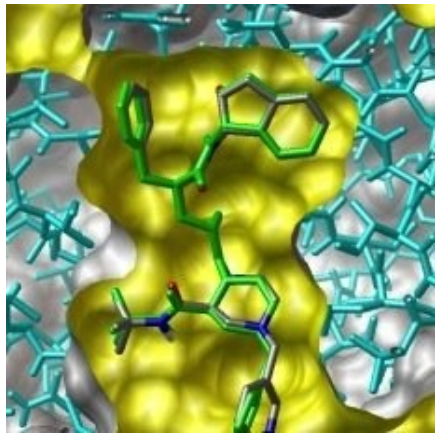
$$n_r = \left(\frac{1 + 2\alpha\,\mathbf{N}/3\epsilon_0}{1 - \alpha\,\mathbf{N}/3\epsilon_0}\right)^{1/2}$$

refractive index

molecular polarizability (e.g., from DFT)

number density (e.g., from MD)







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molecular polarizability
(e.g., from DFT/ML)

number density
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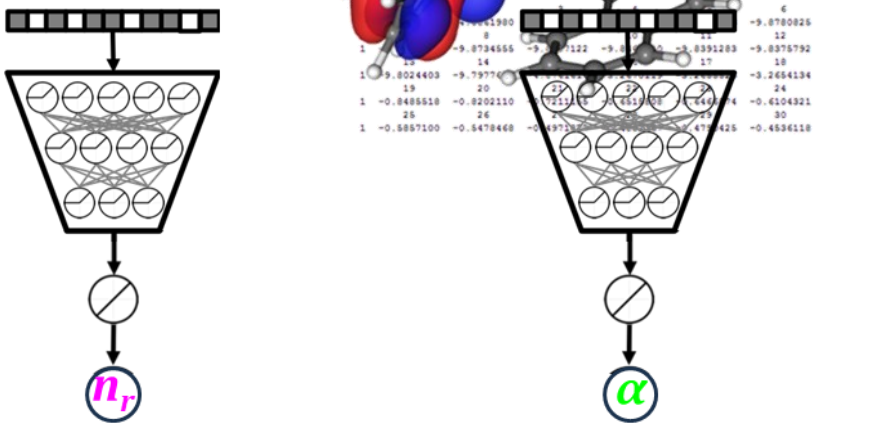




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# Ex: MD number density

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**number density**

- **number density**: $\mathrm{N} = \frac{\rho\, M}{N_A}$



*Chem Sci* 10 (**2019**), 8374.

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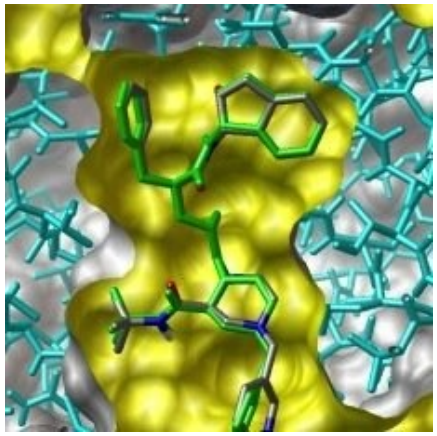
**number density**

- **number density**: $\mathrm{N} = \dfrac{\rho\, M}{N_A}$
  - MD simulation *via* GROMACS
    - difficult and expensive to compute





*Chem Sci* 10 (**2019**), 8374.

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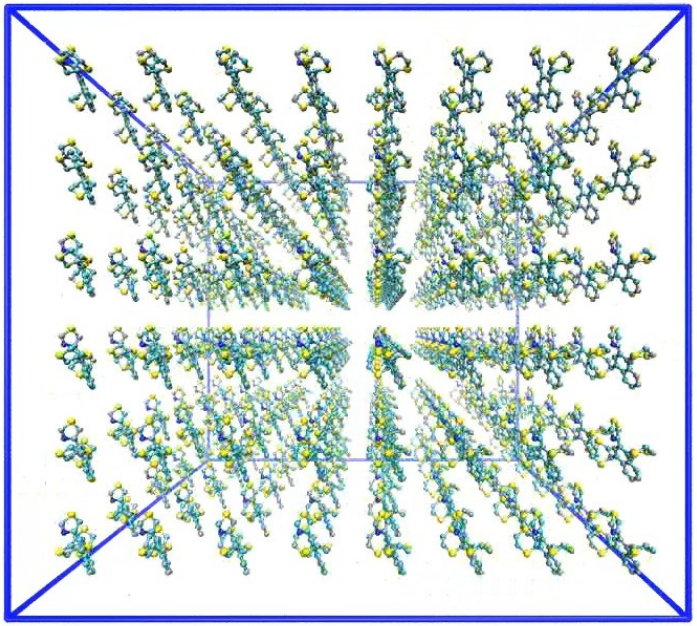

NVT step

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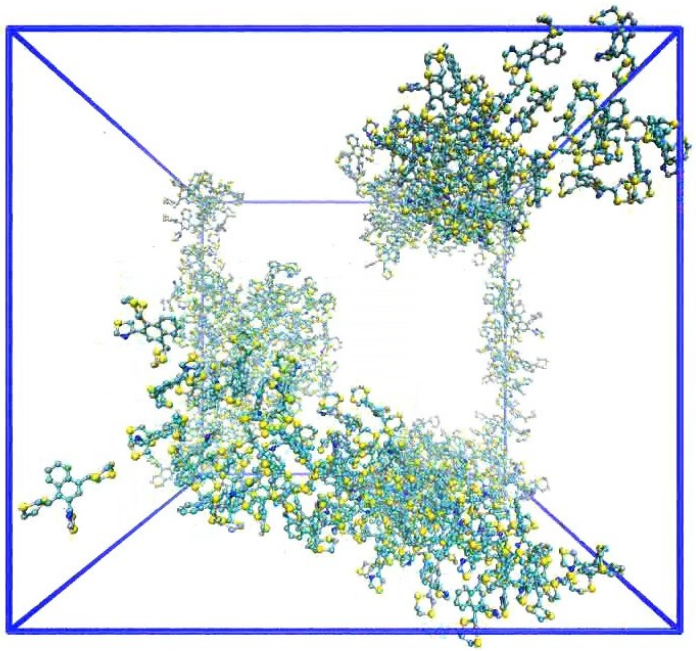

NPT step

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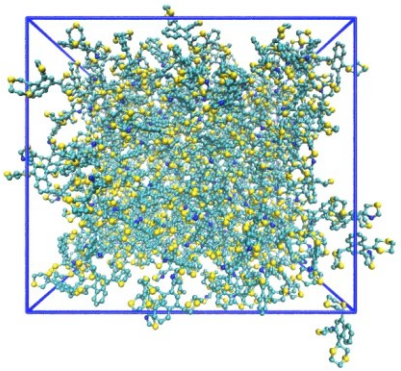

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# Ex: MD number density

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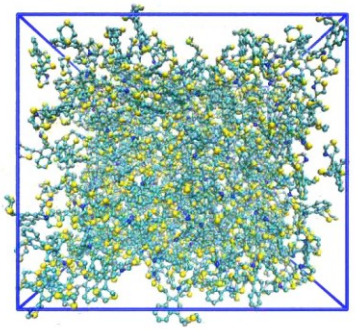

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# Ex: ML model for the MD number density

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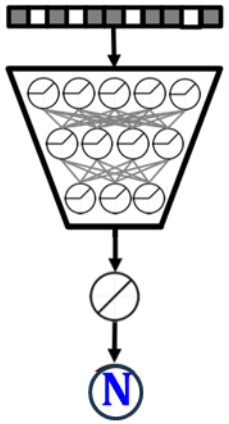


➢ develop an **ML model** for MD results
- DNN regression model

➢ $R^2$ = 0.98, MAPE = 0.9%, RMSPE = 1.1%; i.e., **within intrinsic MD error**

➢ **7 orders of magnitude faster than MD**



*ChemSci* 10 (**2019**), 8374.

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# A WORKING EXAMPLE

Correct physics-based models with data-derived corrections

# Ex: DFT polarizabilities

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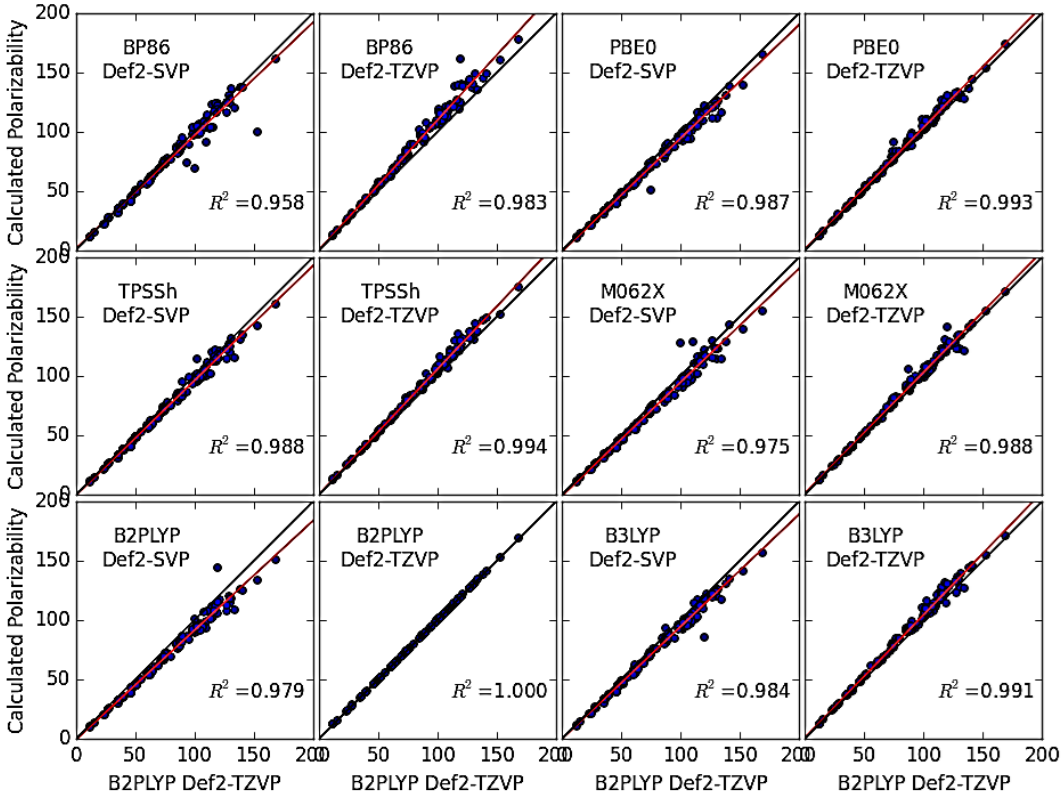
**Lorentz-Lorenz equation**:
(Clausius-Mossotti relation)

$$n_r = \left(\frac{1 + 2\alpha \mathbf{N}/3\epsilon_0}{1 - \alpha \mathbf{N}/3\epsilon_0}\right)^{1/2}$$

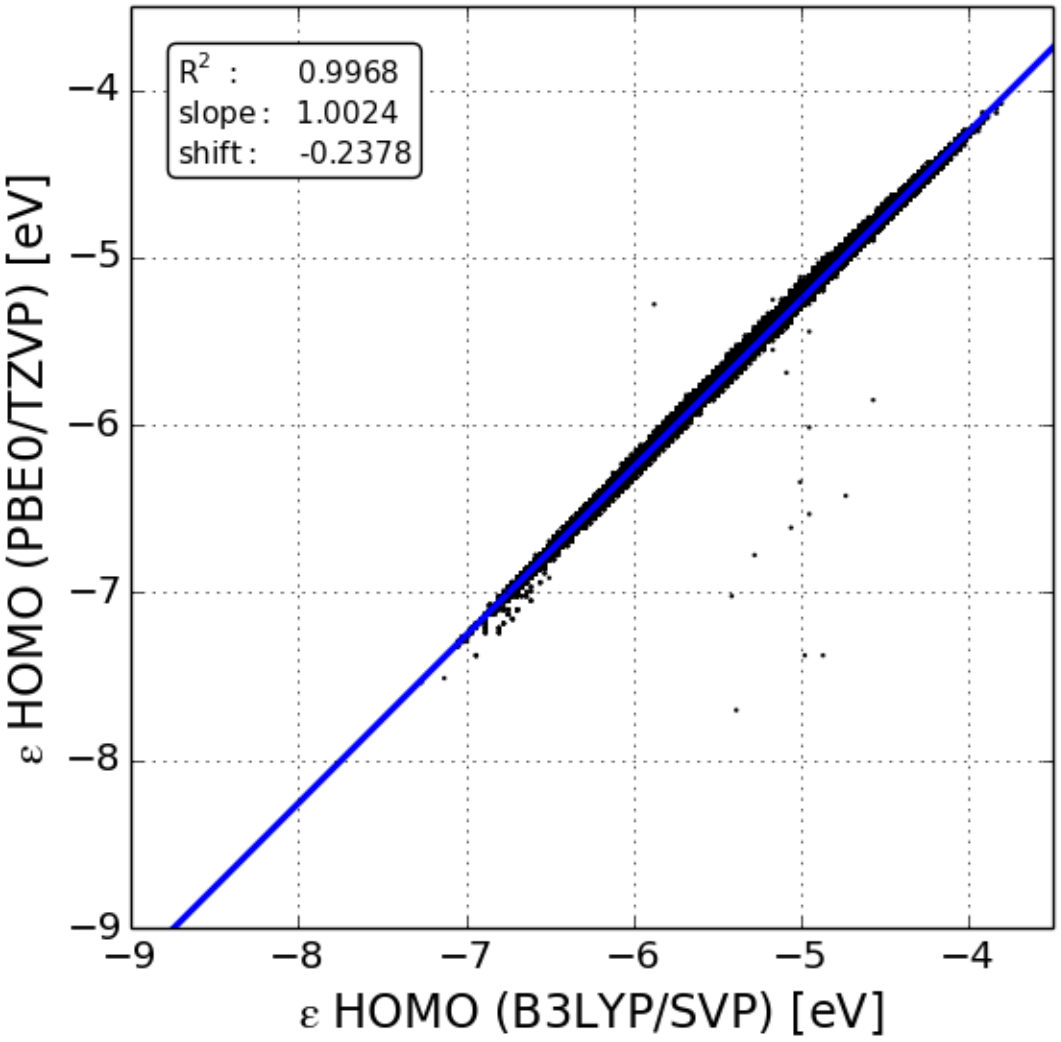
molecular polarizability




*PCCP* 21 (**2019**), 4452.

# Ex: Correcting systematic errors in DFT results






- DZ-hybrid *vs* TZ-hybrid: excellent correlation; straightforward projection

# Ex: Correcting systematic errors in DFT results

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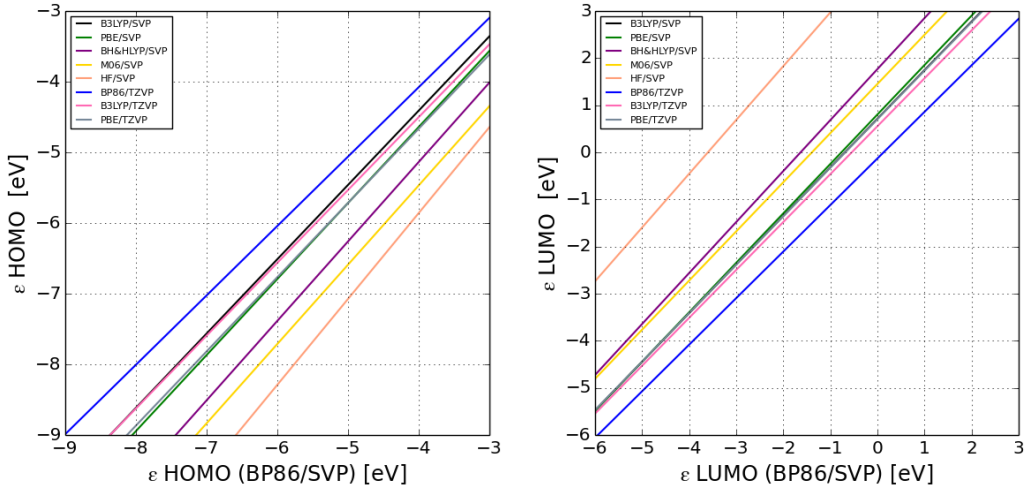
- different physics-based methods yield different data
  - typically, better data is more expensive
  - BUT different data sets are systematically correlated
    - ➢ **exploit by projecting cheap onto expensive data** (e.g., via Δ-learning or transfer learning)






*PCCP* 21 (**2019**), 4452.

# Ex: Correcting systematic errors in DFT results

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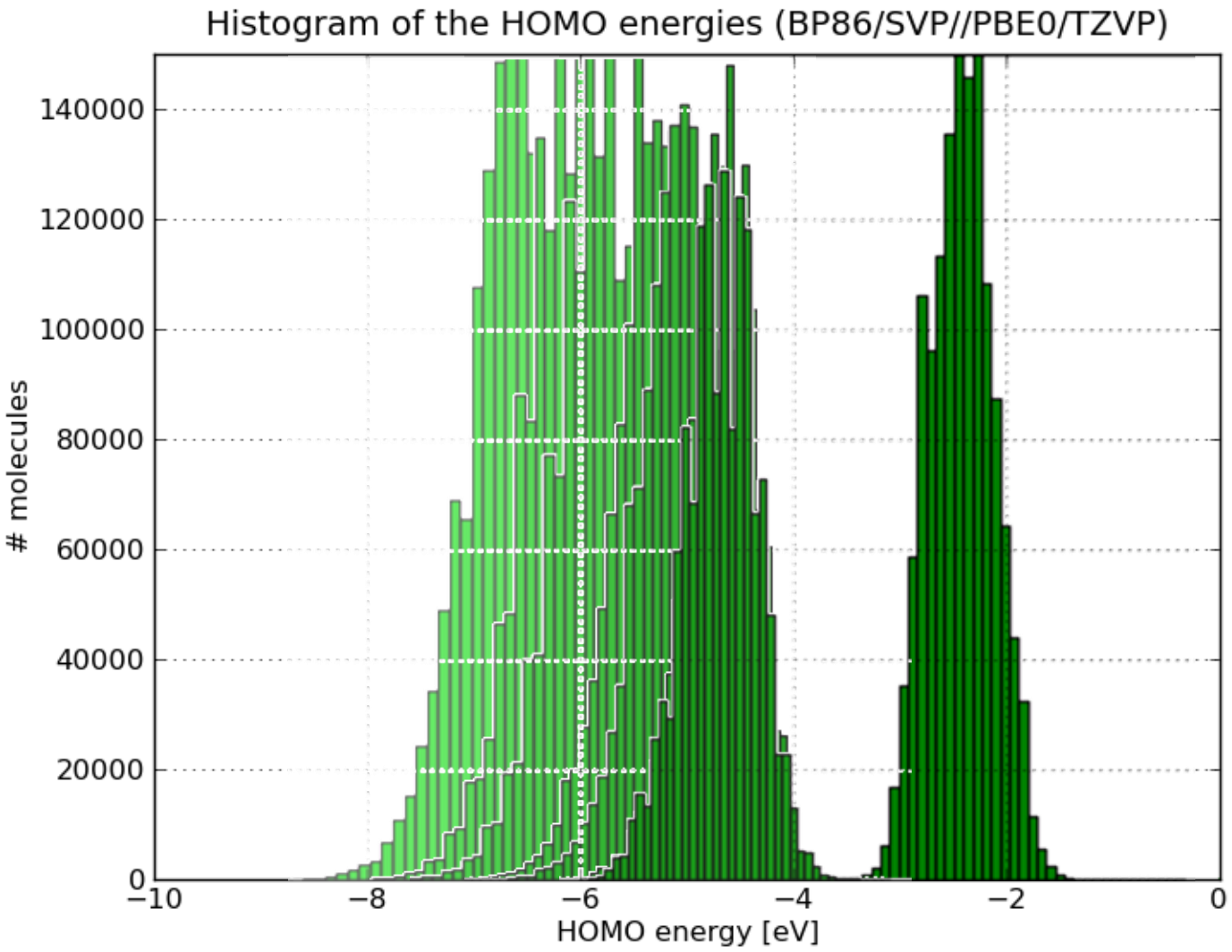


*EES* **7** (**2014**), 698.

# Ex: Correcting systematic errors in DFT results

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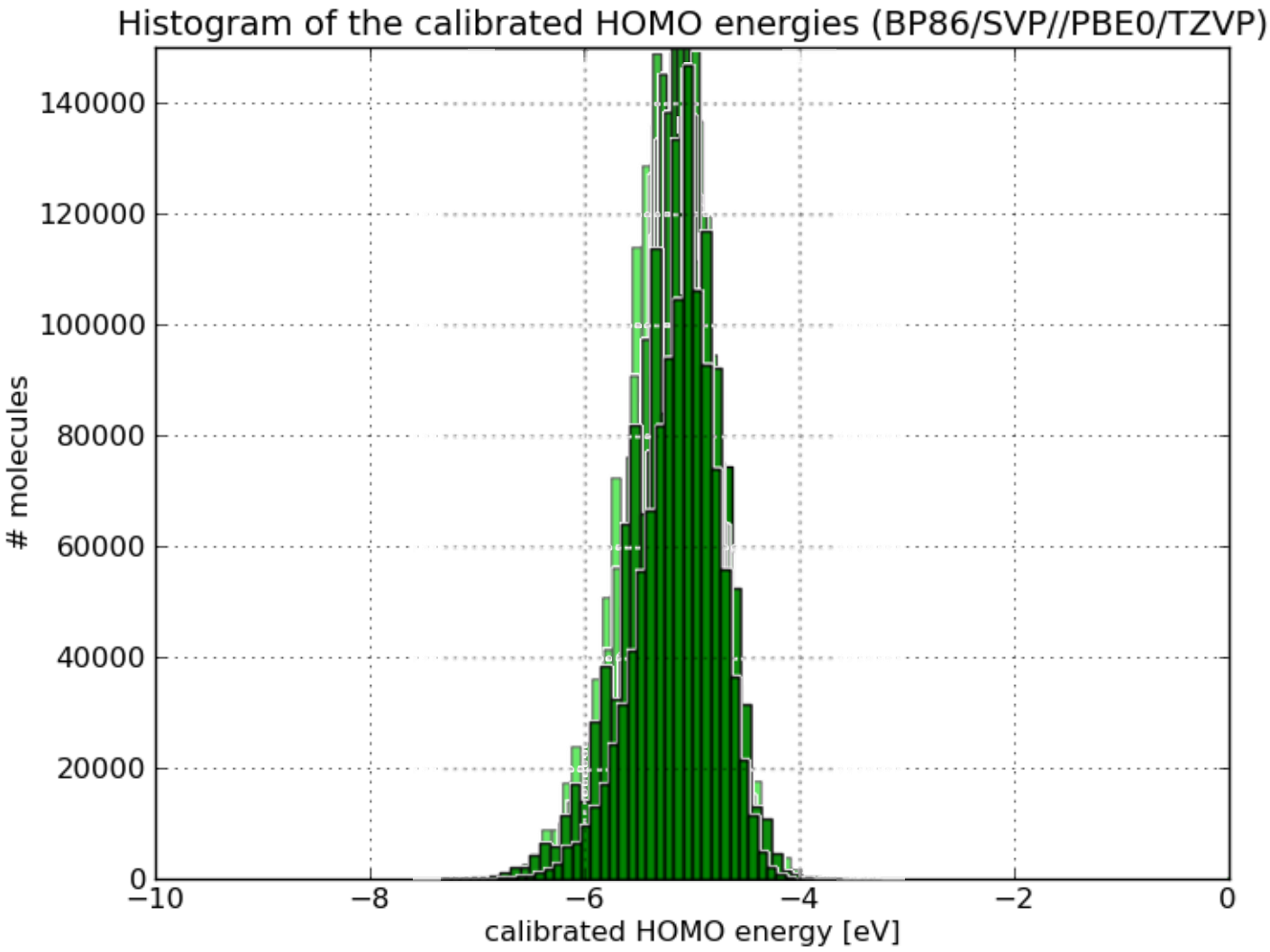


*EES* **7** (**2014**), 698.

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# SO…
# HOW DO WE DO IT?

How to make AI/ML work in the chemistry & materials domain

# How to make AI/ML work in chemistry & materials

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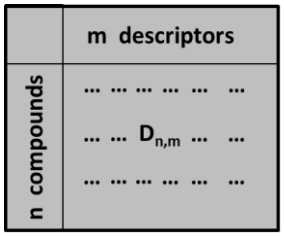
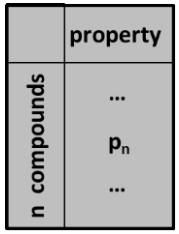
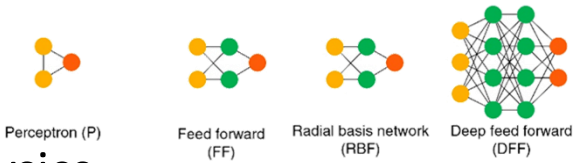
**Challenges for a given problem (… and for the field as a whole)**

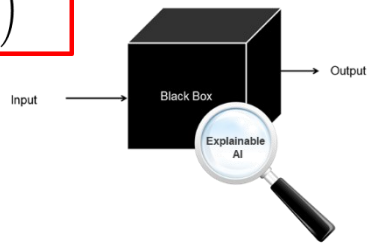
- adequate featurization
  - captures its inherent physics *and* is accessible/affordable
- access to training data of sufficient quality and quantity
  - alternatively: AI/ML for 'small' and/or heteroscedastic data
- identify viable AI/ML approaches
- leverage/incorporate some of the known physics
- explain resulting models and predictions
  - open AI/ML 'black-box', address correlation *vs* causation
- ensure that virtual results are meaningful in the real world
  - e.g., virtually proposed compounds have to be synthetically accessible
  - e.g., AI/ML applicability for extreme value predictions
- realize generative inverse design ideas based on SPR insights
- provide access to all this to community at large

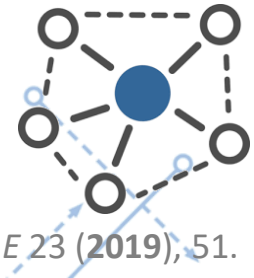



$$n_r = \left(\frac{1 + 2\alpha N/3\epsilon_0}{1 - \alpha N/3\epsilon_0}\right)^{1/2}$$





*COChE* 23 (**2019**), 51.

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# GETTING STARTED WITH ML IN S&E

Important processes and workflows in ML

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# GETTING STARTED WITH ML IN S&E

Python and its important libraries

# Our software ecosystem for data-driven research

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ChemML
0.4.3

Search docs

CHEMML WRAPPER DOCUMENTATION
ChemML Wrapper Tutorial
Input File Manual
Input File GUI
Table of Contents
Wrapper Reference
CHEMML LIBRARY DOCUMENTATION
cheml library



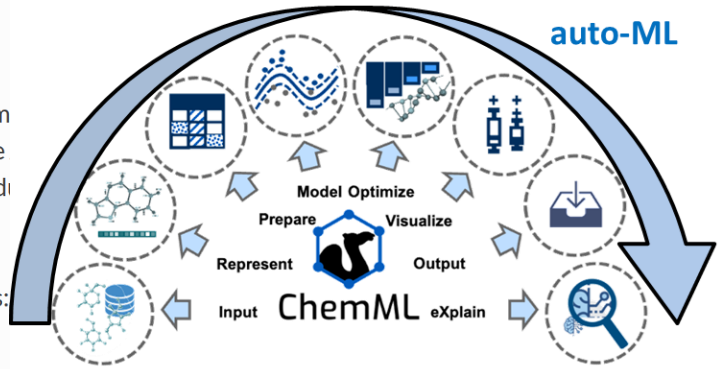

## Welcome to the ChemML's documentation!

ChemML is a machine learning and informatics program suite for the analysis, mining, and modeling of chemical and materials data.

- source: https://github.com/hachmannlab/chemml
- documentation: https://hachmannlab.github.io/chemml

## Code Design:

ChemML is developed in the Python 2 programm
analysis and ML libraries (accessible through the
libraries. The development follows a strictly mod
code as flexible and versatile as possible.




The package consists of two python frameworks:

- **ChemML library (cheml):**

  It is a host for all the methods that are developed or coded from scratch by developers. The format of library is similar to the Scikit-learn library.



*MolSim* 44 (**2018**), 921; *WIRE CMS* (**2020**), e1458; https://github.com/hachmannlab/chemml

# Take-home messages

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AI/ML can become a mainstream tool in chemistry & materials research by…

- … finding patterns in complex data, synthesizing insights;
- … complementing experiment and physical-based models;
- … augmenting, calibrating, or otherwise correcting results;
- … incorporating known physics into data-derived models;
- … guiding studies and their objectives;
- … deepening our understanding of structure-property relationships;
- … accelerating discovery and enabling inverse *de novo* design.


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